8.1 Drift diffusion model

Developing Comsol model

In the following text is summarized the implementation of a model 1D silicon diodes in the program COMSOL Multiphysics in version 3.5. The basic knowledge of working with the program is assumed, so we set out images of important dialogues that define the model. This model is a 1D structure of the doping profile of an identical as in fig. **8.1B.1**. Are implemented equation (8.1B.31) and boundary conditions for ohmic contact (8.1A.37) and (8.1A.41). SRH recombination model and table the value of mobility carriers at 300K is used. To work with this model read the instructions in the layer C.

The diode consist of a line with the coordinates x1 = 0 and $x2 = L = 8 \mu m$. Definition of the necessary constants and expressions is given in fig. 8.1D.1, fig. 8.1D.2 and fig. 8.1D.3.

Name	Expression	Value	Description	
q	1.602e-19[C]	(1.602e-19)[C]	Elementary charge	
Т	300[K]	300[K]	Room temperature	
k	1.38e-23[J/K]	(1.38e-23)[m ² ·kg/(s ² ·K)]	Boltzmanns constant	
epsilon0	8.8541878176e-12	8.854188e-12	Permittivity of vacuum	
epsilonr	11.7	11.7	Rel. permittivity for Si	
ni	1.46e14	1.46e14	Intrinsic concentration for Si	
mun	0.14[m^2/V/s]	0.14[m ² /(s-V)]	Electron mobility for Si	
mup	0.04[m^2/V/s]	0.04[m ² /(s-V)]	Hole mobility for Si	
Dn	k*T/q*mun	0.003618[m ² /s]	Electron diffusivity	
Dp	k*T/q*mup	0.001034[m ² /s]	Hole diffusivity	
taun	0.1[us]	(1e-7)[s]	Electron life time	
taup	0.1[us]	(1e-7)[s]	Hole life time	
u	q/(k*T)	38.695652[s ³ -A/(m ² -kg)]	Reciptrocal thermal voltage	
L	8[um]	(8e-6)[m]	Length of diode	
Lj	1[um]	(1e-6)[m]	Junction length	
с	Lj/sqrt(2*log(Na/Ndi))	(3.295051e-7)[m]	Gauss width constant	
Va	0[V]	0[V]	Applied voltage	
Ndi	1e19[1/m^3]	1e19[1/m ³]	Initial donnor concentration	
Na	1e21[1/m^3]	10e20[1/m ³]	Peak acceptor concentration	
Nd	1e21[1/m^3]	10e20[1/m ³]	Peak donor concentration	
•	1			

Obr. 8.1D.1 Setting of constants

1	Scalar Exp	oressions		×
Name	Expression	Unit	Description	
RSRH	(cn*cp-ni^2)/(taup*(cn+ni)+taun*(cp+ni))	mol/(m ³ -s)	RSRH generation/recombination term	•
n_init	(sqrt(N^2+4*ni)+N)/2	1/m ³	Initial electron concentration	_
p_init	p_init (sqrt(N^2+4*ni)-N)/2 1/m ³ Initial hole concentration			-
psi	1/u*asinh((n_init-p_init)/(2*ni))	0	Initial value of electric potential	
Ν	Ndi + Nd*exp(-((x)/c)^2/2)-Na*exp(-((x-L)/c)^2 $1/m^3$ Fixed charge distribution		-	
4				
OK Cancel Apply Help				
Obr. 8.1D.2 Setting of expressions				

Source Destination				
Boundary selection	Name	Expression	Global destination	
1	lc	q*(ntflux_cp_cd2-ntflux_cn_cd)	v	-
2			×	
			×	
•				
·				
Select by group			v	•
		OK Cancel		

Module Poisson equation

In this section is described the electrostatic module. In fig. 8.1D.4 is depicted the settings of preset formula over the diode domain, where the tab Init is set to psi_init.

🐧 Subdomain Se	ettings - Poisson's Equation (p	ooeq)
Equation		
$-\nabla \bullet (c \nabla psi) = f$		
Subdomains Groups Coeffic	ients Init Element Weak Co	lor/Style
Subdomain selection PDE co	pefficients	
1 Coeff	icient Value/Expression	Description
c	epsilon0*epsilonr	Diffusion coefficient
f	q*(N-cn+cp)	Source term
_		
Group:		
Select by group		
🖌 Active in this domain		
	OK Cancel	Apply Help
Obr. 8.	1D.4 Setting of Poisson equation coefficient	ts

The fig. **8.1D.5** shows the set of boundary conditions at points x_1 and x_2 .

🐠 Boun	dary Settings - Poisson's Equation (poeq)	X
Equation		
h∙psi = r		
Boundaries Groups	Coefficients Weak Color	
Boundary selection	Boundary conditions	
1	 Neumann boundary condition 	
2	Dirichlet boundary condition	
	Coefficient Value/Expression	
	q 0	
	g 0	
	h 1	
Group:	r psi_init	
Select by group		
Interior boundaries		
	OK Cancel Apply H	elp
	a)	
🕫 Boun	dary Settings - Poisson's Equation (poeq)	×
Equation		
h∙psi = r		
	Coefficients Weak Color	
h∙psi = r	Coefficients Weak Color Boundary conditions	
h•pSi = r Boundaries Groups Boundary selection		
h•pSi = r Boundaries Groups Boundary selection	Boundary conditions O Neumann boundary condition	
h•pSi = r Boundaries Groups Boundary selection	Boundary conditions	
h•pSi = r Boundaries Groups Boundary selection	Boundary conditions O Neumann boundary condition O Dirichlet boundary condition	
h•pSi = r Boundaries Groups Boundary selection	Boundary conditions O Neumann boundary condition O Dirichlet boundary condition Coefficient Value/Expression	
h•pSi = r Boundaries Groups Boundary selection	Boundary conditions O Neumann boundary condition Image: Second structure	
h•pSi = r Boundaries Groups Boundary selection 1 2	Boundary conditions Neumann boundary condition Dirichlet boundary condition Coefficient Value/Expression Q 0 g 0	
h•pSi = r Boundaries Groups Boundary selection	Boundary conditions O Neumann boundary condition Image: Dirichlet boundary condition Coefficient Value/Expression Image: Dirichlet boundary condition Image: Dirichlet boundary condition	
h•pSi = r Boundaries Groups Boundary selection 1 2 Group:	Boundary conditions O Neumann boundary condition Image: Dirichlet boundary condition Coefficient Value/Expression Image: Dirichlet boundary condition Image: Dirichlet boundary condition	
h•pSi = r Boundaries Groups Boundary selection 1 2 Group:	Boundary conditions Neumann boundary condition Oefficient Value/Expression q 0 g 0 h 1 r Va+psi_init	
h•pSi = r Boundaries Groups Boundary selection 1 2 Group: Select by group Interior boundaries	Boundary conditions Neumann boundary condition Oefficient Value/Expression Q 0 g 0 h 1 r Va+psi_init	elp

Module convention and diffusion of electrons

In fig. 8.1D.6 is depicted the preset formula over the diode domain, where the tab *Init* is set to *n_init*.

🐧 Subdoma	in Settings - Convection and Diffusion (cd)				
Equation					
$\nabla \bullet (-D \nabla cn + cnu) = R$, cn = concentration					
Subdomains Groups	cn Init Element Color/Style				
Subdomain selection	Species				
1	Library material: Coad				
	Quantity Value/Expression Unit Description				
	D Dn m ² /s Diffusion coefficient				
	R -RSRH mol/(m ³ .s) Reaction rate				
	u mun*psix m/s x-velocity				
	Artificial Diffusion				
Group:					
Select by group					
Active in this domain					
	OK Cancel Apply Help				
Obr. 8.	D.6 Setting of convention and diffusion equations for electrons				

The fig. **8.1D.7** shows identical set of boundary conditions of points x_1 and x_2 .

🤹 Boun	dary Settings - Co	onvection and Diffu	sion (cd)	×
Equation Cn = Cn ₀ Boundaries Groups Boundary selection	dary Settings - Co cn Weak Constr. Boundary conditions Boundary condition: Quantity cn ₀ N ₀ D d	Color	Unit mol/m ³	Description Concentration Inward flux Diffusion coefficient Thickness
Group: Select by group Interior boundaries		OK OK	Cancel	Apply Help

Module convention and diffusion of holes

In fig. 8.1D.8 is depicted the preset formula over the diode domain, where the tab *Init* is set to *p_init*.

🐧 Subdomai	n Settings	- Convection and Diffusion (cd2)			
Equation					
$\nabla \bullet (-D \nabla cp + cp \mathbf{u}) = R, cp = concentration$					
Subdomains Groups	cp Init	Element Color/Style			
Subdomain selection	Species				
1	Library ma	aterial: 🗨 Load			
		Value/Expression Unit Description			
	D	Dp m ² /s Diffusion coefficient			
	R	-RSRH mol/(m ³ -s) Reaction rate			
	u	-mup*psix m/s x-velocity			
	Artificia	I Diffusion			
Group:					
Select by group					
Active in this domain					
		OK Cancel Apply Help			
Obr. 8	3.1D.8 Setting	of convention and diffusion equations for holes			

The fig. **8.1D.9** shows identical set of boundary conditions of points x_1 and x_2 .

🐞 Bound	dary Settings - Co	nvection and Diffus	ion (cd2)	×
Equation				
cp = cp ₀				
Boundaries Groups	cp Weak Constr.	Color		
Boundary selection	Boundary conditions			
1	Boundary condition:	Concentration 🗸	•	
2	Quantity	Value/Expression	Unit	Description
	cp ₀	p_init	mol/m ³	Concentration
	N ₀		mol/(m ² ·s)	Inward flux
	D		m²/s	Diffusion coefficient
▼	d		m	Thickness
Group:				
Select by group				
Interior boundaries				
		ок	ancel	Apply Help
	0 0 (1 1		<i>cc</i> · 11	<i>C</i> 1 1

Obr. 8.1D.9 Setting of boundary conditions for convention and diffusion module of holes

Other settings

Setting of discretization mesh is shown in fig. 8.1D.10 and settings of solver in fig. 8.1D.11.

🚺 Free	Mesh Parameters	×
Global Subdomain Boundary		ОК
Maximum element size:	1e-7	Cancel
Maximum element size scaling factor:		Apply
Element growth rate:	1.3	Help
Reset to Defaults Remesh	Mesh Selected	

Obr. 8.1D.10 Setting of the density discretization mesh

1	Solver Parameters
Analysis types	General Parametric Stationary Adaptive Optimization/Sensitivity Advanced
	OK Cancel Apply Help

Obr. 8.1D.11 Setting of solver parameters